Infrared Absorption Studies of Gypsum under High Pressure

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Introduction: Infrared (IR) spectroscopy continues to be an invaluable tool to study the physical and chemical properties of minerals. In particular, IR spectroscopy is ideal for studying O-H bonding in minerals. Study of the hydrous phases in key minerals provides important insight on the investigation of the dynamics in the earth's mantle. For instance, dehydration, amorphization and other phase transitions in hydrous minerals are linked to the mechanisms of the generation of deep-focus earthquakes.[1, 2]

Methods and Materials: We performed high-pressure IR microspectroscopy of gypsum, $CaSO_4 \cdot 2H_2O$, using Bruker IFS 66v/S spectrometer and IRscopeII system combined with synchrotron source at NSLS beamline U2A. Natural gypsum was compressed up to sub-micrometer film and loaded into the pressure chamber of diamond anvil cell with ruby (as pressure gauge) and KBr (as pressure transmitting medium). Taking the advantage of synchrotron source, i.e. high brightness, high-quality absorption spectra were obtained by measuring transmission of pure KBr (as background) and sample+KBr separately with 20μm×20μm aperture at every pressure.

Results: **Figure 1** shows IR absorption spectra as a function of pressure in O-H stretching mode region. At ambient pressure, four peaks at 3242.6, 3404.3, 3492.5, and 3547.4cm^{-1} (ν_1 to ν_4) were observed, respectively. It can be seen that the patterns of IR absorption change dramatically with increasing pressure. These are related to pressure-induced phase transitions indicated with different colors. Pressure dependence of O-H stretching mode frequencies is shown in **Figure 2**. Bellow 5 GPa, all peaks shift to lower energy except ν_3. Around 5GPa, new vibration modes appear and accompany the frequency discontinuity and change of slope. Similar changes happened again when pressure was reached to about 8.9 and 11.8 GPa, respectively. Theses changes are attributed to phase transitions, which is well consistent with the results of X-ray diffraction experiments.[3] Different phases are clearly distinguished by the discontinuity of frequency and change of slope. Analysis of the new phase structures based on X-ray diffraction, IR absorption and Raman scattering is on the way.

Conclusions: Pressure dependence of the O-H stretching mode patterns/frequencies of gypsum is very sensitive with phase transition. IR absorption spectra reveal that gypsum undergoes three pressure-induced phase transitions at 5.2±0.5, 8.9±0.3, and 11.8±0.4 GPa, respectively. The results are consistent with that of X-ray diffraction.

References: [1] S.H. Kirby, J. Geophys. Res., **92**, 13789 (1987); [2]C. Meade, R. Jeanloz, Science, **252**, 68 (1991); [3]E. Huang, J.A. Xu, J.F. Lin, J. Hu, High Pressure Research, **17**, 57 (2000).

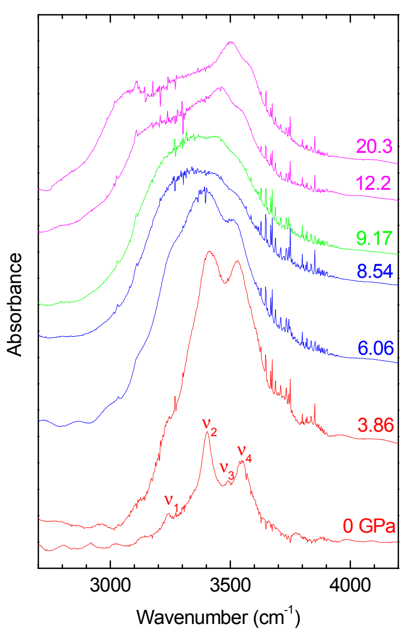

Figure 1. IR absorption spectra of gypsum in O-H stretching region as a function of pressure. Different colors represent different phases.

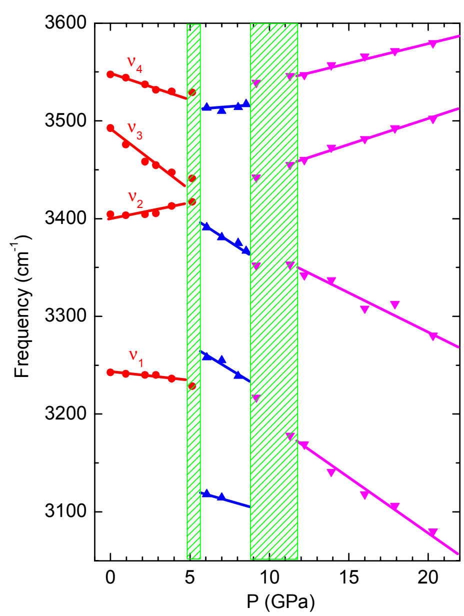

Figure 2. Pressure dependence of O-H stretching mode frequencies. The discontinuity of frequency and slope with pressure is attributed to three new phase transitions.